DTU Library

State Estimation in the Automotive SCR DeNOx Process

Zhou, Guofeng; Jørgensen, John Bagterp; Duwig, Christophe; Huusom, Jakob Kjøbsted

Publication date:
2012

Document Version
Publisher's PDF, also known as Version of record

Citation (APA):
Zhou, G., Jørgensen, J. B., Duwig, C., & Huusom, J. K. (2012). *State Estimation in the Automotive SCR DeNOx Process*. Poster session presented at 8th IFAC Symposium on Advanced Control of Chemical Processes, Singapore, Singapore.

State Estimation in the Automobile SCR $DeNO_x$ Process

Guofeng Zhou, John B. Jørgensen, Christophe Duwig & Jakob K. Huusom

ADCHEM 2012, Singapore

DTU Chemical Engineering
Department of Chemical and Biochemical Engineering

Outline

- Motivation

- Modeling the SCR System
- State Estimation
- Simulation Results

- Conclusions

Motivation

Air quality, especially in urban areas is challenged by exhaust gasses from road vehicles.

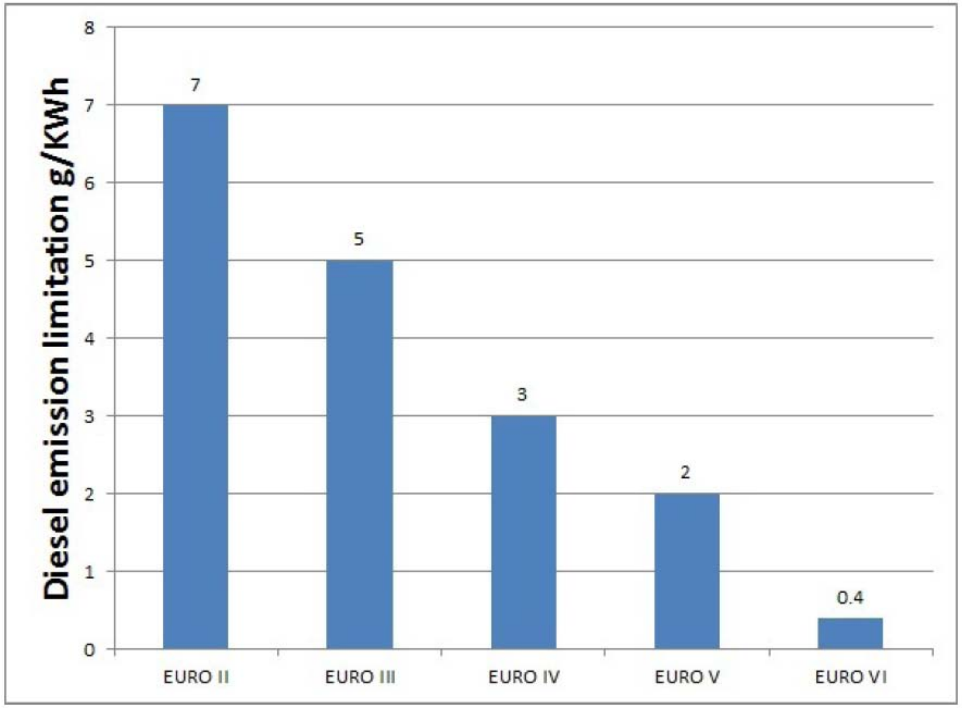
Pollutants such as CO, NO_x and particular matter from vehicles are harmful for the human respiratory system. NO_x further contribute to acid rain, formation of O_3 and smog conditions.

Diesel engine fume has been elevated to ***known carcinogen*** level by W.H.O. on June 12, 2012.

It is estimated that 30 % of the NO_x and 65 % of the particular matter emissions from road vehicles are due to heavy duty diesel vehicles even thou these only comprise only 2 % of the total on road population.

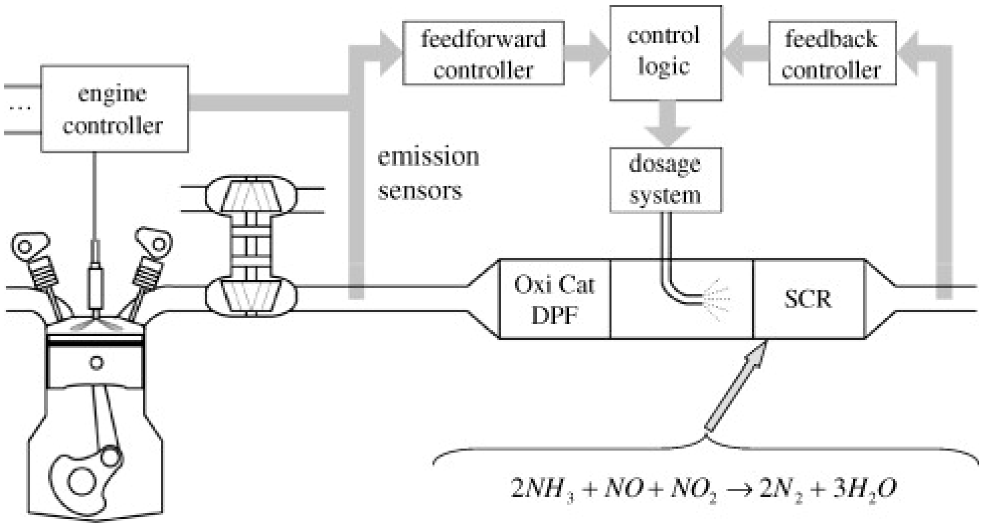
Motivation

Worldwide, legislations are made to gradually reduce emission limits from diesel cars and trucks to counteract these problems.



Efficient exhaust gas after treatment systems exists, but as the limits are reduced more intelligent systems are required.

Diesel engines exhaust gas cleaning system



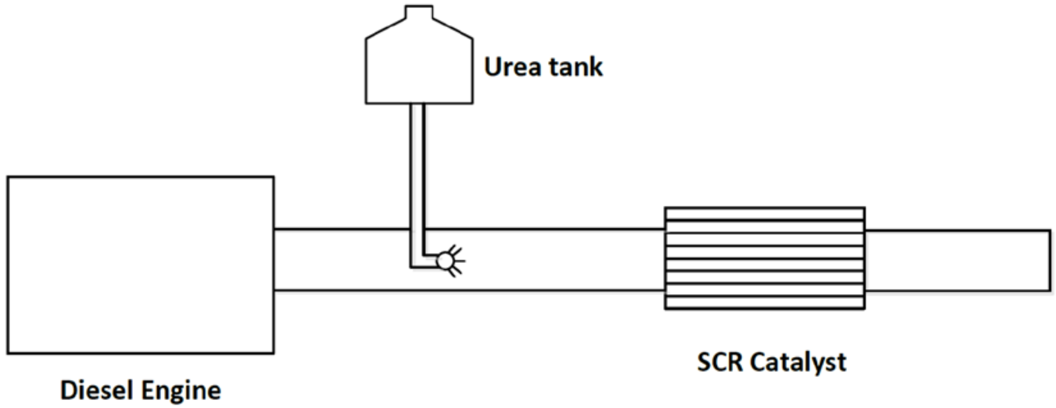
Guzzella 2009, Annual Reviews in Control

Control objectives

Over a full driving cycle an efficient exhaust gas cleaning system will

- Minimize emissions of nitrogen oxides
- Avoid ammonia slip from the catalyst

Modeling the SCR system



Modeling Assumptions:

- The flow in the SCR can be modeled as a CSTR
- Energy balances can be neglected and the system temperature equals the flue gas
- No deactivation of the catalyst
- All chemical reactions temperature dependent assuming an Arrhenius expression for the kinetics constants
- Instantaneous conversion of urea to ammonia

Modeling the SCR system - Chemistry

Adsorption and desorption of ammonia on the catalyst surface

$$NH_3 + (*) \rightleftharpoons NH_3^*$$

$$r_{ads} = k_{ads} C_{NH_3} (1 - \theta_{NH_3})$$

$$r_{des} = k_{des} \theta_{NH_3}$$

Reduction of NO_x (standard SCR reaction)

$$4NH_3^* + 4NO + O_2 \rightarrow 4N_2 + 6H_2O$$

$$r_{red1} = k_{red1} C_{NO} \theta_{NH_3}$$

Reduction of NO_x (fast SCR reaction)

$$2NH_3^* + NO + NO_2 \rightarrow 2N_2 + 3H_2O$$

$$r_{red2} = k_{red2} C_{NO} C_{NO_2} \theta_{NH_3}$$

Ammonia oxidation

$$4NH_3^* + 3O_2 \rightarrow 2N_2 + 6H_2O$$

$$r_{ox} = k_{ox} C_{O_2} \theta_{NH_3}$$

Modeling the SCR system

Component balances over the SCR system

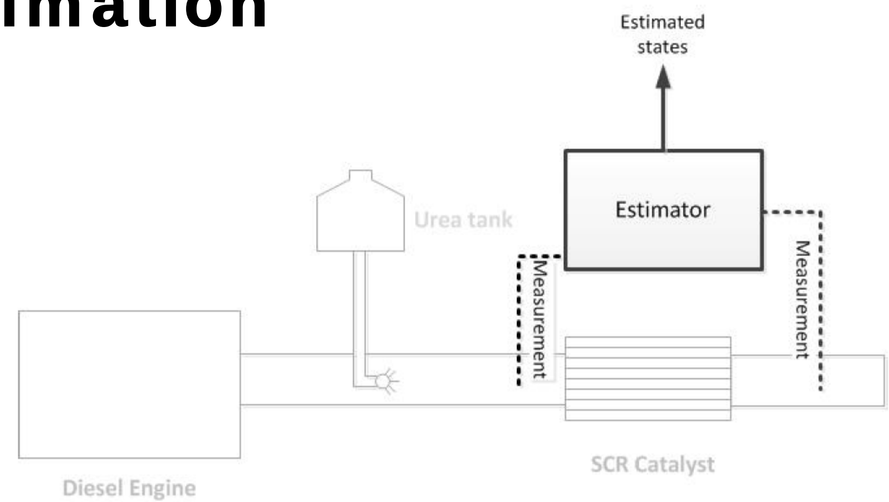
$$\dot{C}_{NO} = {}^{F}/_{V}\left(C_{NO,in} - C_{NO}\right) - 4\Theta k_{red1} C_{NO}\theta_{NH_3} - \Theta k_{red2} C_{NO} C_{NO_2}\theta_{NH_3}$$
$$\dot{C}_{NO_2} = {}^{F}/_{V}\left(C_{NO_2,in} - C_{NO_2}\right) - \Theta k_{red2} C_{NO} C_{NO_2}\theta_{NH_3}$$
$$\dot{C}_{NH_3} = {}^{F}/_{V}\left(C_{NH_3,in} - C_{NH_3}\right) + \Theta k_{des}\theta_{NH_3} - \Theta k_{ads} C_{NH_3}\left(1 - \theta_{NH_3}\right)$$
$$\dot{\theta}_{NH_3} = k_{ads} C_{NH_3}\left(1 - \theta_{NH_3}\right) - k_{des}\theta_{NH_3} - 4k_{red1} C_{NO}\theta_{NH_3} - 2k_{red2} C_{NO} C_{NO_2}\theta_{NH_3} - 2k_{ox} C_{O_2}\theta_{NH_3}$$

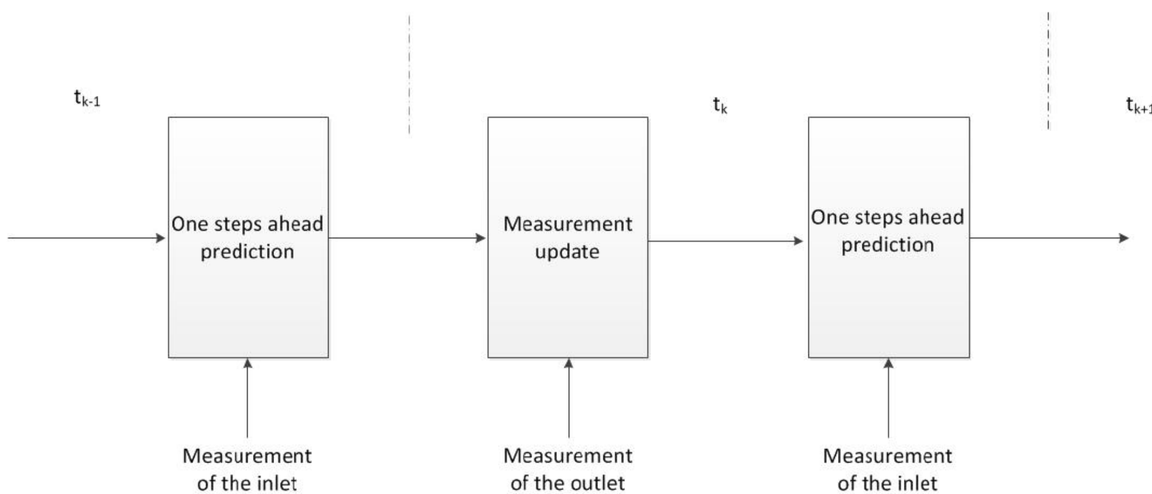
The model result in the following general system of ODE's

$$\dot{x} = f(x(t), u(t), d(t))$$

$$x = \begin{bmatrix} C_{NO} \\ C_{NO_2} \\ C_{NH_3} \\ \theta_{NH_3} \end{bmatrix}, \quad u = C_{NH_3,in}, \quad d = \begin{bmatrix} F \\ T \\ C_{NO,in} \\ C_{NO_2,in} \\ C_{O_2,in} \end{bmatrix}$$

State Estimation





State Estimation – Ordinary Kalman Filter

Discrete time system description

$$x^d_{k+1} = Ax^d_k + Bu^d_k + Ed^d_k + w_k$$
$$y_k = Cx_k + v_k$$

Measurement Update

$$e_k = y^d_k - C\hat{x}^d_{k|k-1}$$
$$K_{f,k} = P_{k|k-1}C^T[CP_{k|k-1}C^T + R_v]^{-1}$$
$$\hat{x}^d_{k|k} = \hat{x}^d_{k|k-1} + K_{f,k}e_k$$
$$P_{k|k} = P_{k|k-1} - K_{f,k}[CP_{k|k-1}C^T + R_v]K^T_{f,k}$$

Time update (one step ahead prediction)

$$\hat{x}^d_{k+1|k} = A\hat{x}^d_{k|k} + Bu^d_k + Ed^d_k$$
$$P_{k+1|k} = AP_{k|k}A^T + R_w$$

State Estimation – Extended Kalman Filter

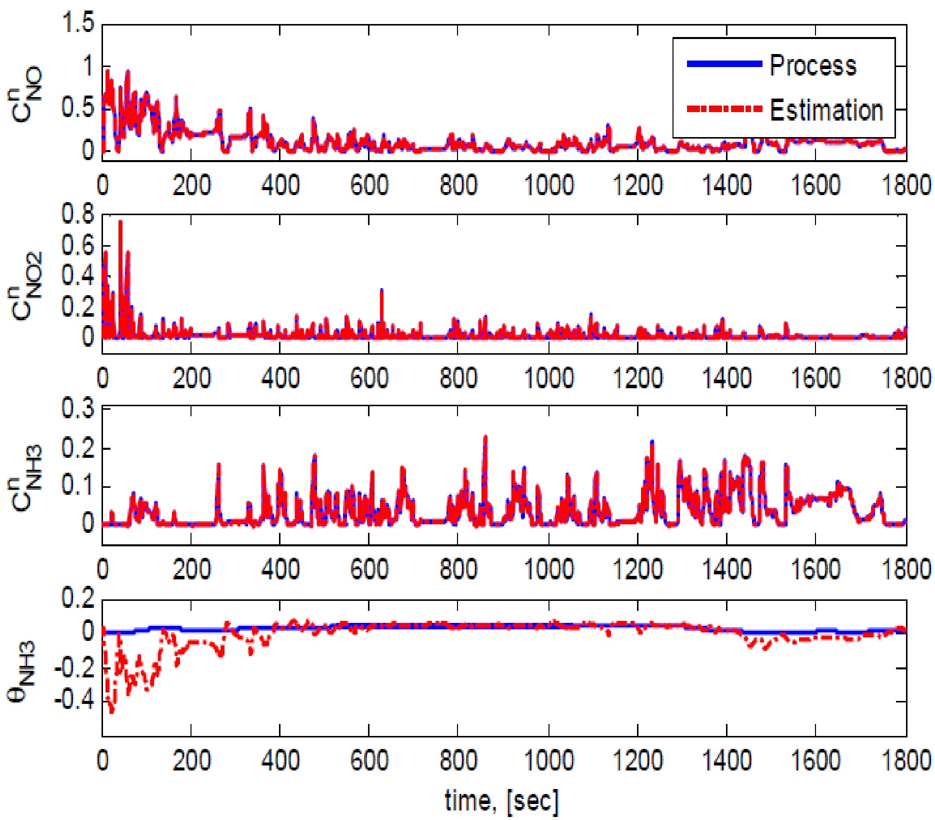
Measurement Update

$$
\begin{aligned}
e_k &= y_k - C\hat{x}_{k|k-1} \\
K_{f,k} &= P_{k|k-1}C^T[CP_{k|k-1}C^T + R_v]^{-1} \\
\hat{x}_{k|k} &= \hat{x}_{k|k-1} + K_{f,k}e_k \\
P_{k|k} &= P_{k|k-1} - K_{f,k}[CP_{k|k-1}C^T + R_v]K_{f,k}^T
\end{aligned}
$$

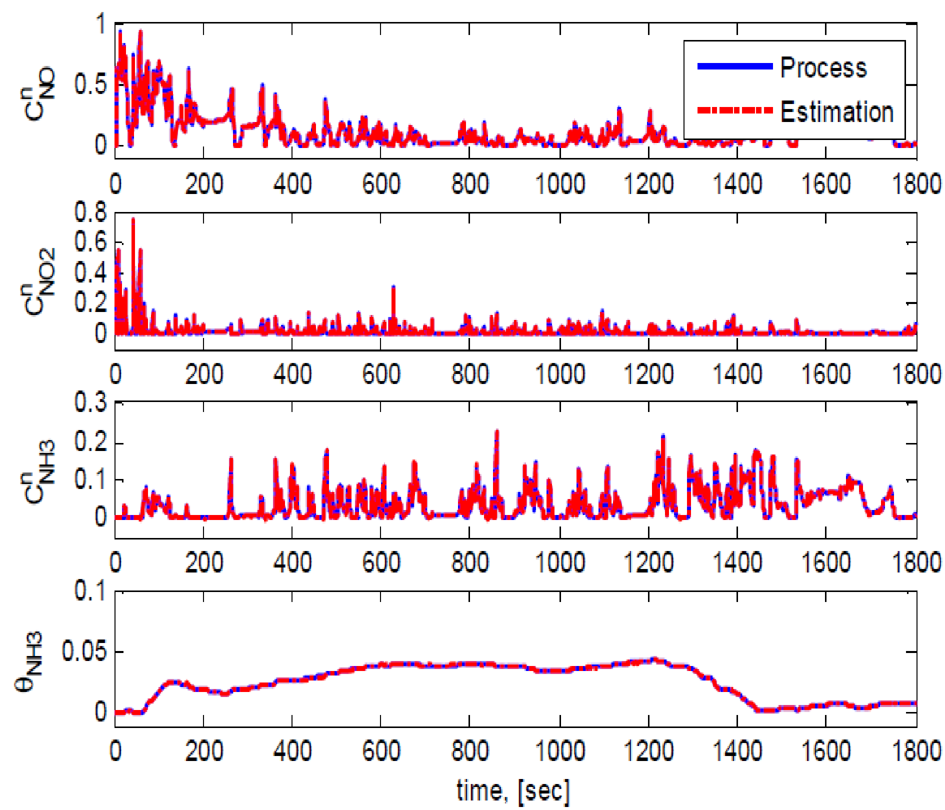
Time update (one step ahead prediction)

$$
\begin{aligned}
\hat{x}_{k+1|k} &= \hat{x}_{k|k} + \int_{t_k}^{t_{k+1}} f(x(\tau), u_k, d_k)d\tau \\
\bar{A}_k &= I + \int_{t_k}^{t_{k+1}} \frac{\partial f}{\partial x}(x(\tau), u_k, d_k)S_{\hat{x}_{k|k}}d\tau \\
P_{k+1|k} &= \bar{A}_k P_{k|k}\bar{A}_k^T + R_w \\
\dot{S}_{\hat{x}_{k|k}} &= \frac{\partial f}{\partial x}(x(t), u_k, d_k)S_{\hat{x}_{k|k}}
\end{aligned}
$$

Simulation Results
Ideal model; NO, NO_2 and NH_3 measurement

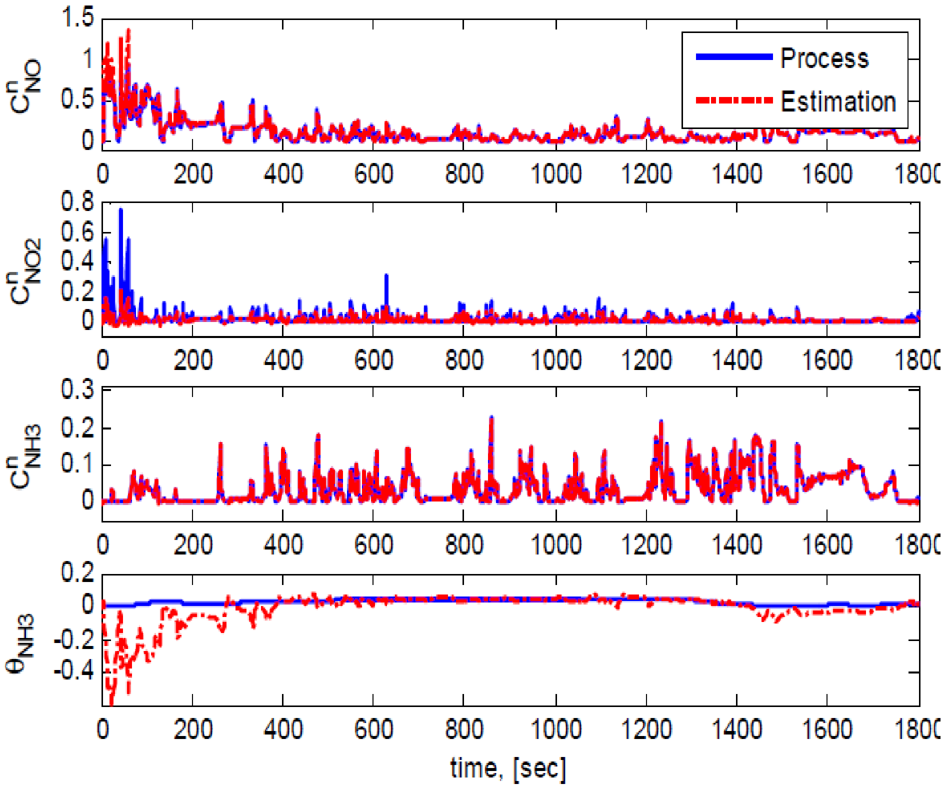


Ordinary Kalman Filter

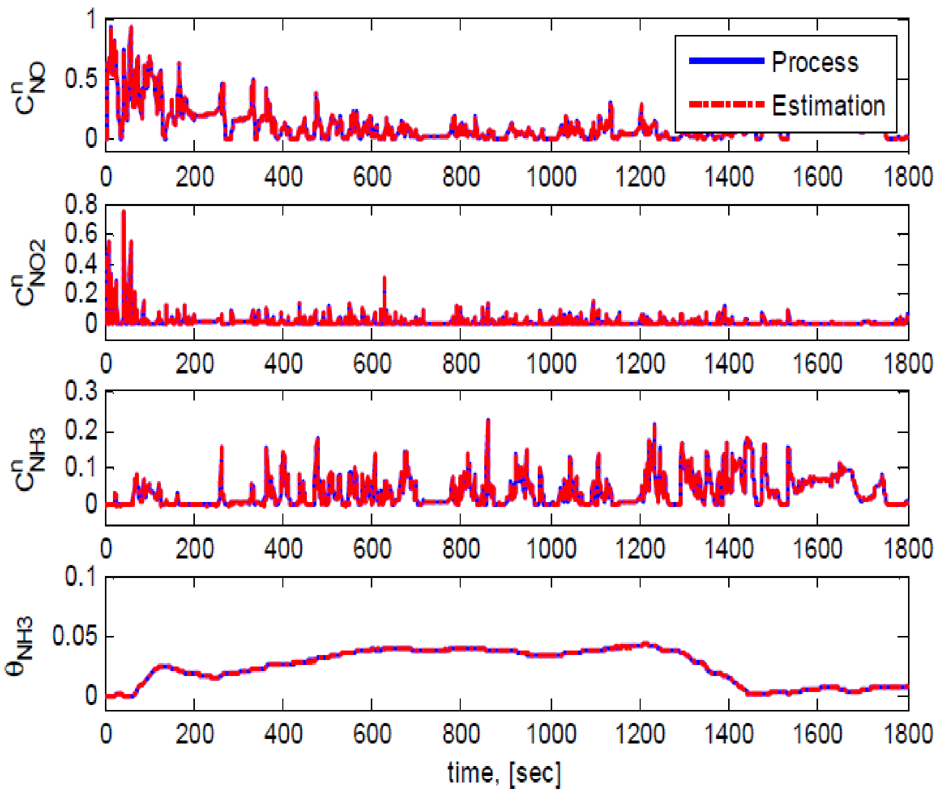


Extended Kalman Filter

Simulation Results
Ideal model; NO_x and NH_3 measurement



Ordinary Kalman Filter



Extended Kalman Filter

Results so far …

We see that the extended Kalman filter clearly outperformed the ordinary formulation for this process, hence it is necessary to include the nonlinear dynamics in the state estimation.

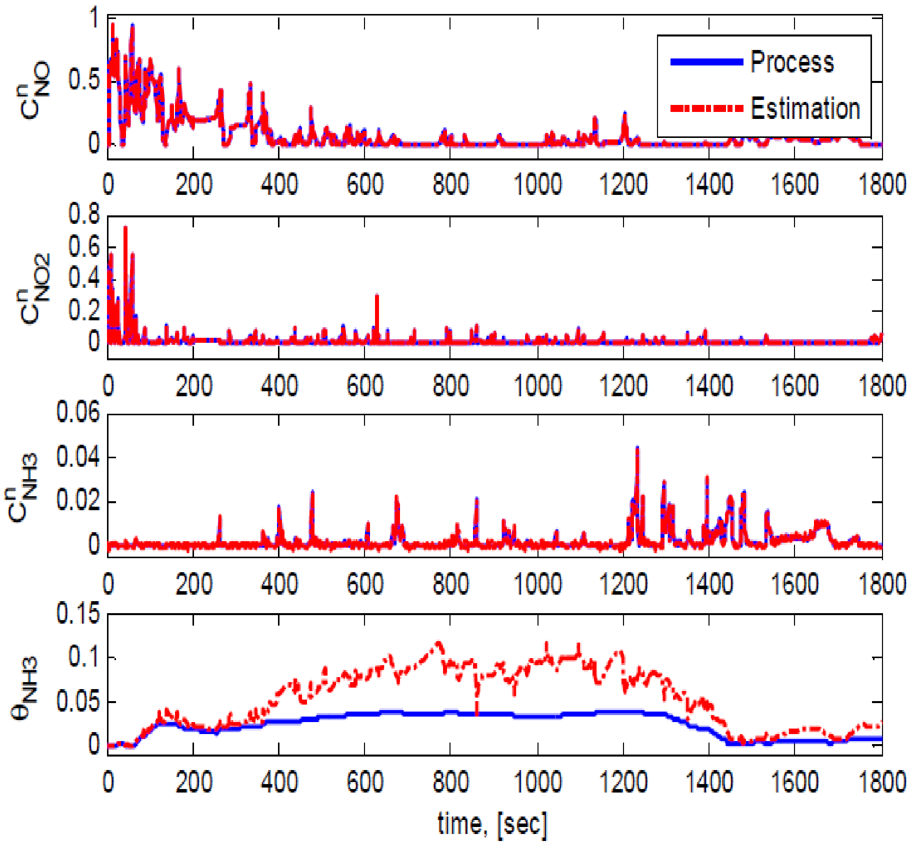
The results so far have been promising, but we also assume perfect model information.

In reality the flow regime is not perfectly well mixed but plug flow with some degree of axial dispersion.

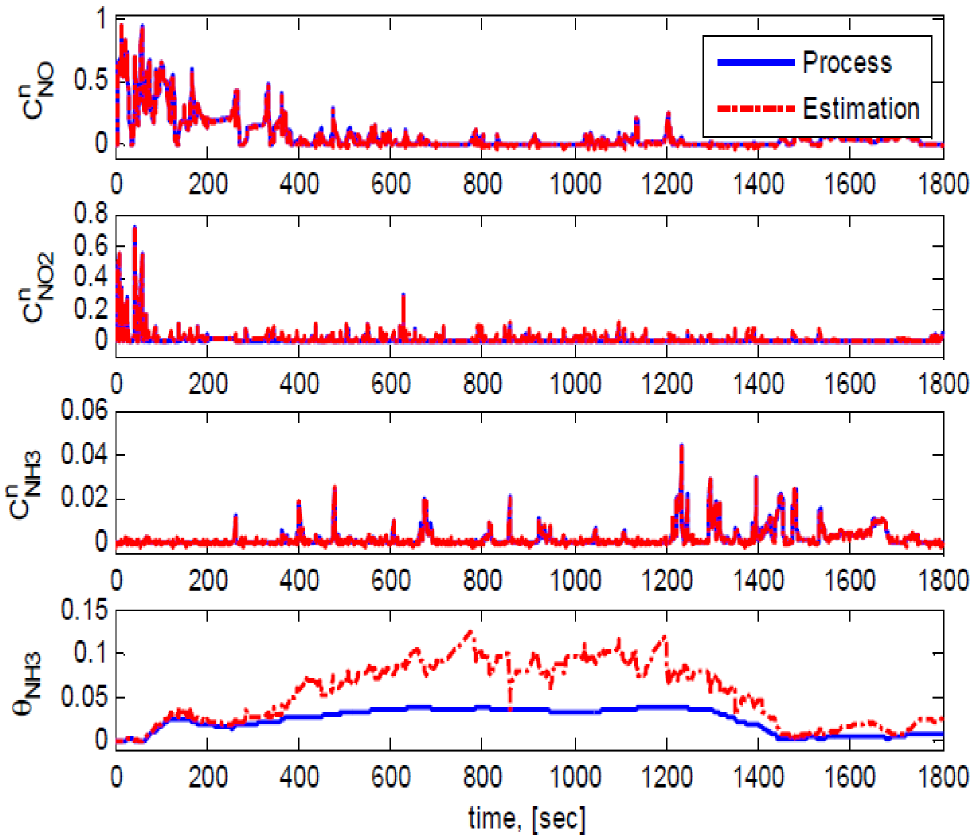
Other assumptions are somewhat questionable too.

- Transport phenomena from the bulk gas to the surface
- Modeling of the catalyst surface temperature

Simulation Results
Under modeling – Extended Kalman Filter



NO, NO_2, NH_3



NO_x, NH_3

Conclusions

A nonlinear filter is necessary to estimate ammonia coverage of the catalyst surface in the SCR unit.

The current model we use has a good level of complexity for fast computations but it lacks some accuracy needed for precise estimates

- Flow
- Surface temperature
- Transport limitations

The proposed filter would be useful in model based control implementations

- Feed forward + simple PI type feedback control
- Model Predictive Control